Renormalized mean-field theory for a two-component Fermi gas with s-wave interactions.

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A method is introduced to renormalize the zero-range interaction for use in mean-field and many-body theory, starting from two-body calculations. The density-renormalized delta-function interaction is then applied using mean-field theory to a two-component fermion gas, and compared with diffusion Monte Carlo simulations and conventional mean-field calculations. In the unitarity limit, the equation of state exhibits the expected behavior $\mu \propto \rho^{2/3}$, with a parameter $\beta = -0.492$, which is consistent with recent experiments[1, 2, 3, 4].

PACS numbers:

I. INTRODUCTION

The low energy scattering of fermionic atoms controls the structure and dynamics of an ultracold quantum Fermi gas. When the scattering length a_0 between fermions in different internal spin states is tunable, for instance, in an external magnetic field, it becomes possible to study the crossover between BCS-type superfluidity of momentum pairs and Bose-Einstein condensation (BEC) of molecules.

In recent years, the BCS-BEC crossover problem has become experimentally accessible [5, 6, 7, 8], enabling sharp tests. The BCS theory has been successful in explaining superfluidity in Fermi gases, but this theory is incomplete because it neglects the Hartree term of the interaction, $4\pi a\rho/m$, where ρ is the density of one spin component. Comparatively little research has considered Fermi gases including the Hartree term, with the primary regime studied being the perturbative case where $\rho a_0^3 << 1$. This is usually referred as the "normal state" of the gas, in contrast with the superfluid state. Quantum Monte Carlo (QMC) simulations include both the Hartree term and pairing physics, but a complete theory that contains both ingredients is still required.

When the range of interaction is much smaller than the inter-particle distance, the potential can be replaced by a delta function interaction although this must be done with caution because the delta function interaction is too singular to be exactly solvable, even in principle. In the weakly-interacting limit, $\rho a_0^3 << 1$, the coupling parameter in the delta function interaction is proportional to the two-body scattering length a_0; this is known as the Fermi pseudo-potential [9]. Using this approximation, mean field theories have been applied to Fermi gases [10, 11]. The use of this approximation in strong interacting regimes leads to an unphysical collapse of the Fermi gas. To go beyond the Fermi approximation for the pseudo-potential, it is crucial to renormalize the coupling constant; the purpose of this paper is to introduce a new and convenient way to achieve this renormalization.

Full diagonalization of a Hamiltonian with delta-function interactions requires a momentum cut-off renormalization even in the weak interacting limit. This type of renormalization has been carried out, for example, in Refs.[12, 13, 14, 15, 16, 17, 18, 19, 20], just to name a few such studies. However, such a renormalization is unnecessary at small or modest scattering lengths, when treated by mean-field theories with zero-range interactions because they are well behaved in this limit. To go beyond the weakly-interacting limit of mean-field theory we propose a density-dependent renormalization of the coupling parameter that is intended to apply even in the long-wavelength limit. A density-dependent renormalization for a 2-component degenerate Fermi gas has been recently proposed in Ref. [21] to explain the stability of this system in the strong interacting limit; a functional form for the effective scattering length a_{eff} was designed to give the expected behavior (i.e. as determined by QMC and other calculations) in both the weak interaction limit and the unitarity limit. Our renormalization strategy is different, in that we present a method to calculate a_{eff} by using the exact energies of two particles in a trap. We compare the many-particle predictions obtained using the renormalized interaction potential with diffusion Monte Carlo and alternative mean-field calculations, and find that our renormalization automatically gives the correct behavior in both the strong and weak interaction limits, for both positive and negative scattering lengths, without imposing this constraint at the outset.

This paper is organized as follows. In Section II we develop the renormalization procedure and show that a simple 2-parameter analytical formula can be utilized to an excellent approximation over the whole range from positive to negative two-body scattering lengths. Section III applies the renormalization to many-particle mean-field theory and presents some of its predictions. Section IV compares the results obtained using our renormalized mean-field theory with quantum Monte Carlo calculations and with perturbative mean-field calculations.

II. RENORMALIZATION PROCEDURE

Through this paper we consider a system of equal mass fermions in a spherically symmetric harmonic oscillator trap at temperature $T = 0$. The Hamiltonian that we

adopt is

$$\mathcal{H} = \sum_i \left(-\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}m\omega^2 \mathbf{r}_i^2 \right) + \sum_{i<i'} \frac{4\pi\hbar^2 a_{eff}}{m}\delta(\mathbf{r}_i - \mathbf{r}_{i'}) \tag{1}$$

This Hamiltonian cannot be diagonalized exactly, since the delta function interaction is too singular and would produce divergent results.[22] The level of approximation we adopt to diagonalize the many-body Hamiltonian is the same we use to solve the corresponding Schrödinger equation for the two-body system. For example, if we want to diagonalize this Hamiltonian in the RPA approximation, we would use RPA for the two-body system and obtain the renormalization through the matching procedure explained later in this Section. An explicitly correlated wavefunction or an extensive configuration interaction (CI) wavefunction can produce divergent results and a momentum cutoff renormalization is necessary. Since we want to obtain and apply a density renormalization without the necessity of introducing a momentum renormalization, we need to carefully select the level of approximation in the wavefunction. The Hartree-Fock (HF) approximation does not introduce explicit interparticle correlations, as the only correlations included are "exchange correlations" from the Pauli exclusion principle. This makes the HF wavefunction a suitable approximation to adopt in our renormalization technique, since it does not require a momentum renormalization.

To obtain the renormalized scattering length we solve (1) for two opposite-spin fermions in the HF approximation. The ground state energies of this approximation are matched with the exact energies of the system for different values of the bare two-body scattering length a_0. From this procedure we extract the functional dependence of a_{eff} on a_0. The spectrum of two opposite-spin fermions in a trap having a specified scattering length a_0 and zero-range interactions can be determined exactly[23, 24, 25, 26] and (1) can be solved numerically for two particles using a Hartree-Fock wavefunction.

Dimensional analysis suggests that, in an infinite, uniform Fermi gas, where the range of the two-body interaction is much smaller than both the average interparticle distance and the bare scattering length a_0, the only parameter that characterizes the behavior of the system is the dimensionless combination $k_f a_0$ of the Fermi momentum and a_0. Throughout this paper the Fermi momentum is defined as $k_f \equiv (6\pi^2\rho)^{1/3}$ where the density is just the one-spin component density. If we were applying the renormalized scattering length a_{eff} to an infinite uniform system, the only relevant parameter would be $k_f a_{eff}$. This suggests that $k_f a_{eff}$ has to be a function of $k_f a_0$. So, we propose the following functional dependence,

$$a_{eff} \equiv \frac{\zeta(k_f a_0)}{k_f} \tag{2}$$

We will see below that the renormalization function, $\zeta(k_f a_0)$, will have the desired behavior in the limiting cases, becoming independent of $k_f a_0$ in the unitarity limit ($|a_0| \to \infty$) and reproducing the relation $a_{eff} = a_0$ in the weak interacting limit ($k_f a_0 \ll 1$). We consider that Eq.(2) holds even with the inclusion of a trapping potential. The renormalized scattering length a_{eff} can be viewed as accounting, in some way, for the correlations neglected in the mean-field wavefunctions.

In choosing to extract a_{eff} from a two-body system, we are implicitly assuming that two-body correlations are the most important in the many-body system. This assumption is reasonable for two-spin component fermions with short-range interactions because the probability of finding more than two fermions close enough to interact is usually negligible.

A. Exact Energies

This subsection reviews the exact results for two particles in a trap interacting through a zero-range pseudopotential. Then, we will select from the energy spectrum, the energy branch that is of interest to study in the renormalization procedure.

Consider two particles of mass m interacting through a two-body potential $V(\mathbf{r})$ in a spherically symmetric trap. If the effective range of the two-body potential is much smaller than the caracteristic length of the trap, the low-lying energy levels depend only on the scattering properties of the potential and not on its shape. Under this condition, the two-body potential can be replaced by a pseudopotential of the form [27]:

$$v(\mathbf{r}) = \frac{4\pi\hbar^2 a(E)}{m}\delta(\mathbf{r})\frac{\partial}{\partial r}r, \tag{3}$$

where $a(E)$ is the energy-dependent scattering length. For ultra-cold gases, the energy dependence on the scattering length can be neglected, so $a(E)$ can be replaced by its energy-independent limit a_0.

Two particles in a trap with this pseudopotential have been considered previously [23, 24, 25, 26]. After separating the center of mass and relative coordinates, the problem reduces to two independent one-dimensional Schrodinger equations. The pseudopotential (3) is introduced as a boundary condition in the relative coordinate Schrodinger equation. The energies are

$$E_{exact} = E_{CM} + E_{rel}, \tag{4}$$

where $E_{CM} = (n_{CM} + 3/2)\hbar\omega$ and

$$\sqrt{2}\frac{\Gamma\left(-\frac{E_{rel}}{2\hbar\omega} + \frac{3}{4}\right)}{\Gamma\left(-\frac{E_{rel}}{2\hbar\omega} + \frac{1}{4}\right)} = \frac{a_{ho}}{a_0} \tag{5}$$

The trap length a_{ho} is defined in this case as $a_{ho} = \sqrt{\hbar/m\omega}$. Equations (4) and (5) reproduce the complete spectrum of the system with zero relative angular momentum. Figure 1 shows the spectrum of E_{rel}

(Eq. (5)) as a function of the scattering length. The lowest curve of the spectrum shown describes the formation of a molecule, where interparticle correlations are fundamental. One anticipates that a HF wavefunction would be a terrible approximation to such a state in which the two atoms are bound together to form a bound molecular eigenstate. Since in this work we do not consider molecule formation, we will consider instead the second branch in Fig. 1 for the renormalization. The renormalization for positive scattering length will only be valid when two-body potential that does not support a bound state. The energies used for the renormalization are $E_{CM} = 3/2\hbar\omega$ and the energy branch where $1/2\hbar\omega < E_{rel} < 5/2\hbar\omega$. This branch of solutions is a smooth curve which gives the correct non-interacting energy at $a_0 = 0$.

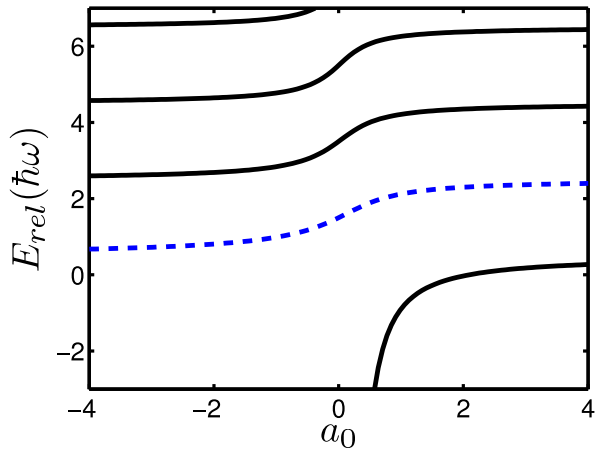

FIG. 1: (Color Online) Spectrum E_{rel} as a function of a_0. The dashed blue line corresponds to the energy branch selected for the renormalization procedure developed in this study.

B. Mean-field solution

Next we determine a renormalization function $\zeta(k_f a_0)$ which, applied to the system of two particles in a trap and using the HF approximation, yields the exact results obtained in the previous section.

To obtain the HF solution of two opposite-spin particles in a trap, we utilize a product wavefunction having the same orbital for both particles. Thus, the two-body spatial wavefunction is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{r}_1)\psi(\mathbf{r}_2) \tag{6}$$

and the spin part is antisymmetric. We introduce this trial wavefunction into the Hamiltonian and obtain the energy functional,

$$\mathcal{E}(\psi) = \int \left(2\psi(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2\mathbf{r}^2\right)\psi(\mathbf{r}) + \frac{4\pi\hbar^2\zeta(k_f a_0)}{mk_f}\psi(\mathbf{r})^4\right) d\mathbf{r}. \tag{7}$$

Minimization of this energy functional determines the ground state energy and wavefunction. The minimization is done with respect to the orbital $\psi(\mathbf{r})$ as in a standard HF procedure.[28] But prior to carrying out this minimization of Eq. (7), we must choose how to evaluate k_f. Since its formal definition is $k_f \equiv (6\pi^2\rho)^{1/3}$, this means that k_f depends at each r-value on $\psi(\mathbf{r})$. For many-particle systems, we would use local density approximation to evaluate k_f. But the application of a local density approximation for a system of two particles does not seem physically correct, so, for two particles we consider the expectation value of $\overline{k}_f$, to be the more appropriate quantity.

$$\overline{k}_f \equiv \int k_f(\mathbf{r})\psi(\mathbf{r})^2 d\mathbf{r} = \int (6\pi^2\psi(\mathbf{r})^2)^{1/3}\psi(\mathbf{r})^2 d\mathbf{r} \tag{8}$$

The minimization procedure leads to a Schrödinger-type equation, where $\psi^2(\mathbf{r})$ is the 1-particle density:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2\mathbf{r}^2 + \frac{8\pi\hbar^2(6\pi^2)^{1/3}\overline{\rho}}{3m}\left(\frac{\zeta'(\overline{k}_f a_0)a_0}{\overline{k}_f} - \frac{\zeta(\overline{k}_f a_0)}{\overline{k}_f^2}\right)\psi(\mathbf{r})^{2/3} + \frac{4\pi\hbar^2\zeta(\overline{k}_f a_0)}{m\overline{k}_f}\psi(\mathbf{r})^2\right)\psi(\mathbf{r}) = \epsilon\psi(\mathbf{r}) \tag{9}$$

where ϵ is a Lagrange multiplier which represents the chemical potential. The relation between ϵ and the energy is not as straightforward as in the HF case, owing primarily to the appearance of $\zeta'(k_f a_0)$. It should be understood that $\psi(r)^{2/3}$ is supposed to be evaluated on a branch for which it is real and positive everywhere. Here and in the following, $\zeta'(x) \equiv d\zeta(x)/dx$.

Equation (9) corresponds to the GP equation for 2 particles with a renormalized scattering length $a_{eff} = \zeta(\overline{k}_f a_0)/\overline{k}_f$. After solving Eq.(9) we use (7) to evaluate the energy. The basic idea is, for any chosen bare two-body scattering length a_0, to find $\zeta(\overline{k}_f a_0)$ so that the energy of the ground state of (7) matches exactly the appropriate energy of (4). From our numerical experience, the functional dependence of ζ on $\overline{k}_f a_0$ appears to be uniquely defined by the set of equations (4, 5, 7, 8) and (9).

There are two self-consistent procedures involved in this calculation. To solve Eq. (9) we follow the standard HF procedure, in which we adopt noninteracting solutions as the initial guess for the orbitals, after which we iterate Eq. (9) until convergence is achieved. For this procedure, we need the functional form of $\zeta(\overline{k}_f a_0)$ and

$\zeta'(\overline{k}_f a_0)$ over a range of $\overline{k}_f a_0$ values since $\overline{k}_f$ is changing in each iteration. This means that we cannot find the exact renormalization function $\zeta(\overline{k}_f a_0)$ at any fixed value of a_0 without knowledge of the functional form of $\zeta(\overline{k}_f a_0)$ at nearby values. To solve this problem we calculate $\zeta(\overline{k}_f a_0)$ self-consistently over the *entire* range in $\overline{k}_f a_0$ that is of interest. First we select a set of scattering length a_0 values which cover the entire range of interest. For an initial trial dependence $\zeta^{(0)}(\overline{k}_f a_0)$ we solve Eqs. (9) and (7) at each a_0, obtaining the energy E, $\overline{k}_f$, the wavefunction and ϵ. Then, to obtain a new $\zeta^{(1)}(\overline{k}_f a_0)$, we look for the value of scattering length $\widetilde{a}_0$ for which $E_{exact}(\widetilde{a}_0) = E$, and we generate a new renormalization function that satisfies $\zeta^{(1)}(\overline{k}_f \widetilde{a}_0) = \zeta^{(0)}(\overline{k}_f a_0)$. The modification of the renormalization function is evidently in the abscissa rather than in the ordinate. This is a convenient way to approach this calculation. Once we have carried out the matching procedure onto the whole set of scattering length a_0 values, we generate the next iteration for $\zeta^{(1)}(\overline{k}_f a_0)$ and its derivative by interpolation.

In the next iteration, $\zeta^{(0)}(\overline{k}_f a_0)$ is replaced by $\zeta^{(1)}(\overline{k}_f a_0)$ and we repeat the energy matching step for the whole set of a_0-values. This procedure is repeated a few times until it converges to give a single correct renormalization function function $\zeta(\overline{k}_f a_0)$. Note that this iterative procedure determines a "numerically exact" renormalization function $\zeta(\overline{k}_f a_0)$. Because the iteration procedure is efficient, in 5 iterations we obtain 9 digits of agreement between E_{exact} and E over the entire a_0 range. It is important to introduce a sensible initial trial renormalization function $\zeta^{(0)}(\overline{k}_f a_0)$. Many trial $\zeta^{(0)}(\overline{k}_f a_0)$ functions, like $\zeta^{(0)}(\overline{k}_f a_0) = \overline{k}_f a_0$, would produce collapse of the two-fermion wavefunction for large and negative a_0. To avoid this collapse, we propose an initial trial $\zeta^{(0)}(\overline{k}_f a_0)$ which is close to the correct $\zeta(\overline{k}_f a_0)$, this is done by choosing a qualitatively correct functional form with a few free parameters and we then find the set of parameters that best reproduce the exact two-body energies.

The final numerical results obtained for the renormalization function $\zeta(\overline{k}_f a_0)$ are accurately approximated by the monotonic functional form $\zeta_0(\overline{k}_f a_0) = A + B\arctan(C + D\overline{k}_f a_0)$, where A and B are chosen to have the corresponding maximum and minimum values at $a_0 \to \pm\infty$ and C and D are chosen to obey $\zeta(\overline{k}_f a_0) \to \overline{k}_f a_0$ for $\overline{k}_f a_0 << 1$. The maximum value is $\zeta^{max} = 2.182$ and value is $\zeta^{min} = -1.392$, this leads to $A = 0.395$ and $B = -1.138$. To get the correct behavior for $\overline{k}_f a_0 << 1$, this in turn requires $C \equiv \arctan(-A/B) \approx 0.362$ and $D \equiv -(1+C^2)/B \approx -0.994$. Thus there are only two independent parameters A, B to be specified at this level of approximation. Figure 2 compares our numerical results for $\zeta(\overline{k}_f a_0)$ with this arctangent approximation,

$$\zeta_0(\overline{k}_f a_0) = 0.395 - 1.138\arctan(0.362 - 0.994\overline{k}_f a_0). \quad (10)$$

Figure 3 displays the fractional error in $\zeta_0(\overline{k}_f a_0)$ defined as $(\zeta(\overline{k}_f a_0) - \zeta_0(\overline{k}_f a_0))/\zeta(\overline{k}_f a_0)$, showing a maximum error of approximately 5%.

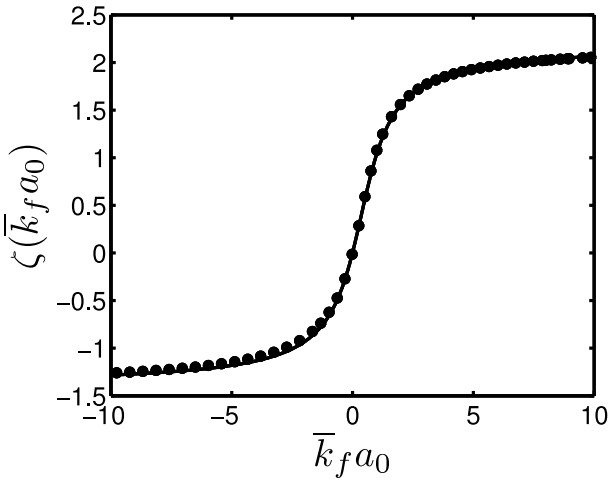

FIG. 2: Effective scattering length $\zeta(\overline{k}_f a_0)$ (circles) and its analytical approximation $\zeta_0(\overline{k}_f a_0)$ (full line)

TABLE I: Exact numerical values of $\zeta(x)$.

x	$\zeta(x)$	x	$\zeta(x)$	x	$\zeta(x)$
$-\infty$	-1.392	-1.6582	-0.82404	4.9199	1.9248
-11.937	-1.2818	-1.3097	-0.73716	5.2872	1.9426
-11.394	-1.2767	-0.96693	-0.62355	5.6545	1.9581
-10.85	-1.2712	-0.63317	-0.47254	6.0219	1.9717
-10.306	-1.2651	-0.31351	-0.27173	6.3892	1.9838
-9.7626	-1.2584	-0.014329	-0.014242	6.7566	1.9946
-9.2193	-1.251	0.26087	0.2863	7.1239	2.0042
-8.6758	-1.2428	0.51684	0.59122	7.4913	2.0129
-8.1326	-1.2336	0.76339	0.86101	7.8586	2.0208
-7.5895	-1.2231	1.0072	1.0787	8.226	2.028
-7.0467	-1.2113	1.2507	1.2474	8.5933	2.0346
-6.504	-1.1977	1.6166	1.4309	8.9607	2.0406
-5.9617	-1.182	1.9829	1.5585	8.0056	2.0238
-5.4197	-1.1635	2.3497	1.6508	8.9117	2.0398
-4.8782	-1.1416	2.7166	1.7201	9.523	2.04896
-4.3373	-1.1153	3.0837	1.7737	9.8669	2.0536
-3.7973	-1.0829	3.4509	1.8164	10.895	2.0657
-3.2585	-1.0423	3.8181	1.8512	11.311	2.0699
-2.7216	-0.99004	4.1853	1.88	11.998	2.0763
-2.1875	-0.92043	4.5526	1.9042	$+\infty$	2.182

Now that the renormalization function has been determined, other observables can be tested for the two particle system. Interestingly, there is a numerically exact agreement between the the external trap potential energy expectation values measured with the exact wavefunction and with the mean-field renormalized wavefunction. However, the one-particle density profiles calculated using the exact wavefunctions and the mean-field renormalized wavefunction are only in qualitative agreement,

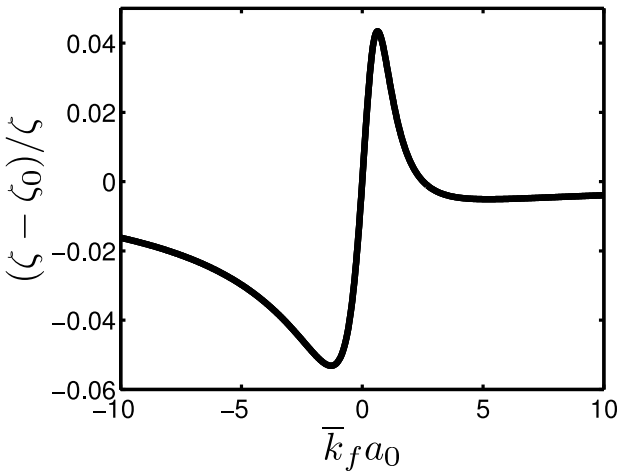

FIG. 3: Fractional error in our analytical approximation to the numerical renormalization function, $\zeta_0(\overline{k}_f a_0)$.

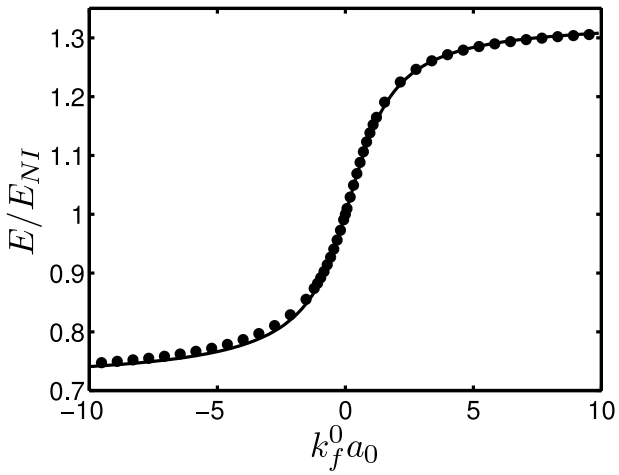

FIG. 4: Ratio of the total energy to the non-interacting energy, for a spherically-trapped two-component degenerate Fermi gas in the large N limit. The circles correspond to HF calculations for 2280 particles using $\zeta(k_f a_0)$, while the solid line corresponds to either the variational solution, eq. (16), or the TF solution, eq. (25), (the curves are indistinguishable on the scale of the figure) using the approximate renormalization function $\zeta_0(k_f a_0)$.

e.g. for scattering lengths of large magnitude, where $|\overline{k}_f a_0| >> 1$.

III. APPLICATION TO MANY-PARTICLE SYSTEMS

This section presents different many-particle approximations for which the renormalized scattering length can be used. The renormalization procedure is designed to be used in the Hartree-Fock approximation, however we will see that simpler approximations like Thomas-Fermi (TF) or a variational trial wavefunction will yield equally effective results in the large N limit. The variational wavefunction we will use is the noninteracting wavefunction rescaled in the radial direction by a factor λ as in Eq.(11), where λ is the variational parameter. As an example, we can see in Figure 4 a comparison for the ground state energy of a two-component Fermi gas in an spherical trap in the large N limit. The result obtained with the approximate $\zeta_0(k_f a_0)$ in conjunction either with a variational trial wavefunction or else with the TF method are in good agreement with the full HF calculation with the exact $\zeta(k_f a_0)$. The difference between the results is mainly used by the replace of the exact $\zeta(k_f a_0)$ by the approximate $\zeta_0(k_f a_0)$. If we use the exact $\zeta(k_f a_0)$ for all the methods, the energies agree in at least 3 digits. In systems having a small number of particles, the HF method is, of course, most reliable.

A. Variational

The simplest approximation [29] utilizes a trial wavefunction that is a simple radial rescaling of the noninteracting wavefunction:

$$\Psi_\lambda(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \frac{1}{\lambda^{3N/2}} \Psi_{NI}(\mathbf{r}_1/\lambda, \mathbf{r}_2/\lambda, ..., \mathbf{r}_N/\lambda) \tag{11}$$

The expectation value of the renormalized Hamiltonian (1) can be separated into two terms, $E(\lambda) = E_{HO}(\lambda) + E_{int}(\lambda, a_0)$, where

$$E_{HO}(\lambda) = \langle \Psi_\lambda | \sum_i \left(-\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m\omega^2 \mathbf{r}_i^2 \right) | \Psi_\lambda \rangle$$

$$E_{int}(\lambda, a_0) = \langle \Psi_\lambda | \sum_{i<i'} \frac{4\pi\hbar^2 a_{eff}}{m} \delta(\mathbf{r}_i - \mathbf{r}_{i'}) | \Psi_\lambda \rangle . \tag{12}$$

The energy of this trial wavefunction is calculated as a function of the variational scale parameter λ for the renormalized Hamiltonian (1). The non-interacting wavefunction is a Slater determinant formed with the occupied spin-orbitals. The E_{HO} is simple to calculate, as it requires only a change of variables to determine the λ-dependence in Eq. 12 in conjunction with the known results of the non-interacting ground state.

$$E_{HO}(\lambda) = E_{NI} \left(\frac{1}{2\lambda^2} + \frac{\lambda^2}{2} \right) \tag{13}$$

The interaction energy E_{int} can be written in the following form, when we apply the renormalization locally as a function of the density:

$$E_{int}(\lambda, a_0) = \frac{4\pi\hbar^2}{m} \int \frac{\zeta(k_f^\lambda(\mathbf{r}) a_0)}{k_f^\lambda(\mathbf{r})} \rho_\lambda^2(\mathbf{r}) d\mathbf{r} \tag{14}$$

In this equation ρ is the density of one spin component and $k_f^\lambda(\mathbf{r}) \equiv (6\pi^2\rho_\lambda(\mathbf{r}))^{1/3}$. In the large N limit, the density of the non-interacting wavefunction can be replaced by the TF density of the noninteracting system [30]. The density corresponding to our trial wavefunction is a simple radial rescaling, whereby the density in the high-N limit is:

$$\rho_\lambda(\mathbf{r}) = \begin{cases} \frac{\sqrt{6N}}{3\pi^2 a_{ho}^3 \lambda^3}\left(1 - \frac{r^2}{2a_{ho}^2\lambda^2(3N)^{1/3}}\right)^{3/2} & , \text{ if } r^2 < R_c^2 \\ 0 & , \text{ otherwise} \end{cases} \tag{15}$$

Here N is the total number of particles and $R_c = \sqrt{2}a_{ho}\lambda(3N)^{1/6}$ is the radius of the Fermi gas. In the large N limit, the total energy can be expressed in units of the noninteracting energy,

$$E/E_{NI} = \frac{1}{2\lambda^2} + \frac{\lambda^2}{2} + \frac{1}{\lambda^2}F\left(\frac{k_f^0 a_0}{\lambda}\right). \tag{16}$$

Here λ is the scaling parameter, $k_f^0 = \sqrt{2}(3N)^{1/6}/a_{ho}$ is the Fermi momentum of the non-interacting system at the trap center, and F is

$$F(\gamma) = \frac{4^4}{9\pi^2}\int_0^1 (1-x^2)^{5/2}x^2\zeta\left(\gamma\sqrt{1-x^2}\right)dx. \tag{17}$$

This function must be calculated numerically unless further approximations are made. The energy results obtained using Eq. (16) are shown in Figure 4. In the unitarity limit, the behavior can be calculated exactly:

$$F(\gamma \to -\infty) = \frac{4^4\zeta^{min}}{9\pi^2}\int_0^1 (1-x^2)^{5/2}x^2dx = \frac{5\zeta^{min}}{9\pi}. \tag{18}$$

Three curves predicted by Eq. (16) are shown in Fig. 5. For the entire range of interactions, the energy of the system (the minimum of the curve) remains finite, ranging from $0.713E_{NI}$ to $1.33E_{NI}$, This shows how our renormalization circumvents the collapse that would occur for the bare Fermi pseudopotential.

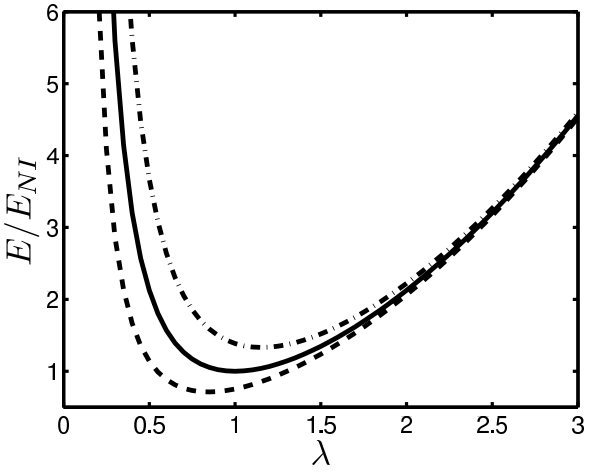

FIG. 5: Total energy as a function of λ, in units of the noninteracting total energy. The solid curve corresponds to $k_f^0 a_0 = 0$, the dashed curve corresponds to $k_f^0 a_0 = -\infty$, and the dotted-dashed curve corresponds to $k_f^0 a_0 = \infty$. The minimum of the energy functional for $k_f^0 a_0 = -\infty$ occurs at $\lambda = 0.844$, which represents the ratio between the cloud radius at unitarity and the noninteracting cloud radius.

B. Thomas-Fermi results

In this subsection we will review the TF approximation, using the renormalization function. The TF approximation has been used to study a 2-component Fermi gas with zero-range pseudo-potentials [31], but no renormalization has been considered.

Thomas-Fermi is of course a local density approximation. At each position inside the trap, the wavefunction is approximated by a Slater determinant of a set of plane wave orbitals, i.e., the orbitals are characterized by four quantum numbers, the vector momentum $\mathbf{k}$ and the spin. The orbitals are filled uniformly up to a level $k_f(r)$ which is the same for spin up and spin down fermions. The value of $k_f(r)$ will depend on the distance r from the trap center, and on the number of particles in the system. For a uniform system, the value of k_f is a constant that characterizes the density of the system.

To calculate the local energy we need to sum over all the states at that position. For example, the kinetic energy term K for one-spin component is:

$$\begin{aligned} K &= \frac{1}{2m}\sum_{\mathbf{k}}\langle\mathbf{k}|\mathbf{p}^2|\mathbf{k}\rangle = \frac{\hbar^2}{2m}\sum_{\mathbf{k}}\mathbf{k}^2\langle\mathbf{k}|\mathbf{k}\rangle \\ &= \frac{V\hbar^2}{2m(2\pi)^3}\int k^2 d^3k = \frac{V\hbar^2}{20\pi^2 m}k_f^5 \end{aligned} \tag{19}$$

Here V is the volume of integration which will disappear when we consider the local energy. This volume is small in comparison with the external potential (in this case the trap) characteristic length but is big enough to contain many particle. So, k_f and V_{ext} can be considered constant during the integration. The calculation of the expectation value of an external trapping potential is then straight forward and we obtain

$$\langle V_{ext}\rangle = \frac{V}{6\pi^2}V_{ext}k_f^3, \tag{20}$$

which is just the number of particles times the external potential at that position. In the case of the interaction term, the two different spin components can be calculated by considering the particles as indistinguishable, and calculating the direct and exchange terms. But since the interaction is a delta function, we can consider the particles as distinguishable with interactions only between different species and obtain the same result. This latter procedure is easier and we only need to consider

the direct term.

$$\langle V_{int}\rangle = \sum_{\mathbf{kk'}} \langle \mathbf{kk'}|V_{int}|\mathbf{kk'}\rangle$$
$$= \frac{1}{(2\pi)^6}\frac{4\pi a_{eff}\hbar^2}{m}\int_0^{k_f}\int_0^{k_f}\int\int \delta(\mathbf{x}-\mathbf{x}')d\mathbf{x}'d\mathbf{x}d^3k'd^3k$$
$$= V\frac{4\pi a_{eff}\hbar^2}{m}\frac{k_f^3}{6\pi^2}\frac{(k_f)^3}{6\pi^2} = V\frac{4\pi\hbar^2}{m}\frac{k_f^5\zeta(k_f a_0)}{(6\pi^2)^2} \quad (21)$$

For the case of two equally-numerous spin components the local energy (per unit volume) is

$$\mathcal{E}(k_f) = E(k_f)/V = \frac{\hbar^2}{2m}\frac{k_f^5}{5\pi^2} + V_{ext}\frac{k_f^3}{3\pi^2} + \frac{4\pi\hbar^2}{m}\frac{k_f^5\zeta(k_f a_0)}{(6\pi^2)^2}. \quad (22)$$

In an infinite uniform system, where $V_{ext} = 0$, the energy is:

$$\mathcal{E}(k_f) = \frac{\hbar^2}{2m}\frac{k_f^5}{5\pi^2} + \frac{4\pi\hbar^2}{m}\frac{k_f^5\zeta(k_f a_0)}{36\pi^4}. \quad (23)$$

The ratio between the total energy and the non-interacting energy has a simple form and only depends on $k_f a_0$,

$$\mathcal{E}(k_f)/\mathcal{E}_{NI}(k_f) = 1 + \frac{10\zeta(k_f a_0)}{9\pi}. \quad (24)$$

Using Eq. 22, we can construct our energy functional by integrating the local energy over all space.

$$E = \int d\mathbf{r}\left(\frac{\hbar^2}{2m}\frac{k_f(\mathbf{r})^5}{5\pi^2} + V_{ext}(\mathbf{r})\frac{k_f(\mathbf{r})^3}{3\pi^2} + \frac{4\pi\hbar^2}{m}\frac{k_f(\mathbf{r})^5\zeta(k_f a_0)}{36\pi^4}\right) \quad (25)$$

To find the ground state we have to minimize the energy under the constraint that the number of particles is fixed. This constraint can be implemented by introducing a Lagrange multiplier μ_0, usually called the chemical potential. So, the minimization of Eq. (25) for fixed number of particles is reduced to the minimization of

$$\Lambda \equiv E - \mu_0 N = E - \mu_0\int d\mathbf{r}\frac{k_f(\mathbf{r})^3}{3\pi^2}, \quad (26)$$

where variational parameter is $k_f(\mathbf{r})$. The necessary but not sufficient condition for $k_f(\mathbf{r})$ to minimize Λ is that

$$\frac{\partial\Lambda}{\partial k_f(\mathbf{r})} = 0. \quad (27)$$

This condition leads to a relationship between the local chemical potential, defined as $\mu(\mathbf{r}) \equiv \mu_0 - V_{ext}(\mathbf{r})$, and the local Fermi momentum $k_f(\mathbf{r})$,

$$\mu(\mathbf{r}) = \frac{\hbar^2 k_f^2(\mathbf{r})}{2m}\left(1 + \frac{10}{9\pi}\zeta(k_f(\mathbf{r})a_0) + \frac{k_f(\mathbf{r})a_0}{18\pi^2}\zeta'(k_f(\mathbf{r})a_0)\right). \quad (28)$$

The value of μ_0 fixes the number of particles and, with this relationship, we can calculate the density profile and the energy of the system. Figure 6 shows the chemical potential dependence on $k_f a_0$ obtained with the renormalization function and with other models. In Figure 4 we can see the energy obtained using eqs. (25,28) in the large N limit.

In the unitarity limit, $a_0 \to -\infty$, we obtain

$$\mu = \frac{\hbar^2 k_f^2}{2m}\left(1 + \frac{10}{9\pi}\zeta^{min}\right) \quad (29)$$

At unitarity, when the scattering length is much larger than the inter-particle distance, the only relevant parameter is the density [32, 33]. Dimensional analysis suggests that $\mu \propto \rho^{2/3} \propto k_f^2$. The expected relation between μ and k_f is usually written as

$$\mu = \frac{\hbar^2 k_f^2}{2m}(1+\beta). \quad (30)$$

From our calculations this relations appears naturally with a coefficient β, which is an universal parameter, of $\beta = 10\zeta^{min}/9\pi = -0.492$. This parameter β has been studied from many different perspectives. Table II shows different experimental and theoretical values of β. Interestingly, our β value is consistent with most experiments. To measure β experimentally, Hulet and Thomas groups measure the size of the cloud and compares it with the noninteracting cloud. For, example, the result obtained by Hulet group is $R_U/R_{NI} = 0.825 \pm 0.02$ which compares well with ours $R_U/R_{NI} = 0.844$ (Fig. 5), obtained using both variational or TF calculations we obtain.

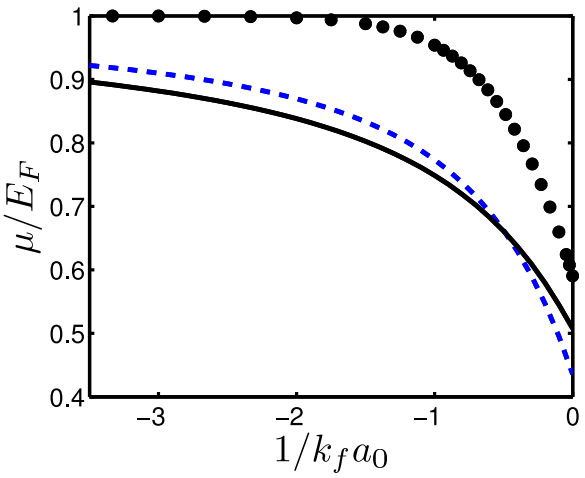

FIG. 6: (Color Online) Chemical potential in units of the Fermi energy. The black solid line is the prediction obtained with the renormalization function. The black circles represent the BCS prediction and the blue dashed curve is the prediction obtained in Ref. [34]

.

It is well established [33, 42, 43] that an ultracold two-component Fermi system exhibits superfluidity. Even

TABLE II: Experimental and theoretical predictions of β.

	β		
Experiments	$-0.54(5)^a$	$-0.64(15)^b$	$-0.49(4)^d$
Experiments	$-0.68^{+0.13\,c}_{-0.10}$	$-0.54^{+0.05\,e}_{-0.12}$	
QMC	$-0.58(1)^f$	$-0.56(1)^g$	
Padé asymptotes	-0.674^h	-0.432^i	
Green's function	-0.545^j	-0.599^k	
BCS	-0.41^l		
Other methods	-0.3^m	-0.564^n	-0.492^o

[a]Ref. [1]
[b]Ref. [2]
[c]Ref. [35]
[d]Ref. [3]
[e]Ref.[4]
[f]Ref. [36]
[g]Ref. [37]
[h]Refs.[32, 38]
[i]Ref.[38]
[j]Ref.[39]
[k]Ref.[40]
[l]This is a well known result, see for example Ref.[39]
[m]Ref.[41]
[n]Ref.[34]
[o]Result obtained in this paper with the renormalization function.

though our renormalization scheme does not explicitly consider superfluidity, it reproduces a number of properties of the Fermi gas sensibly, including the equation of state and the chemical potential. Consequently, these results can be used in the hydrodynamic theory to extract information about dynamics of the system, like the speed of sound or normal modes of excitation. For example, the speed of sound in a uniform two-component system is given by [32]

$$v^2 = \frac{\hbar}{m}\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial E/N}{\partial\rho}\right). \tag{31}$$

Using Eq. (24) we can thus evaluate the speed of sound, which generates the results shown in Figure 7. The speed of sound results reproduce the expected limiting behaviors. In the noninteracting limit $v = v_f/\sqrt{3}$, while at unitarity $v = v_f\sqrt{(1+\beta)/3}$ [44]. This is one example of a nontrivial observable quantity for this system that can be predicted by this renormalization technique. A comprehensive study of other observables based on this approach will be left for future publications.

C. Hartree-Fock method

The HF method for a many-particle system is an extension of the two particle calculation done in Section II. The variational parameters are the orbitals and the

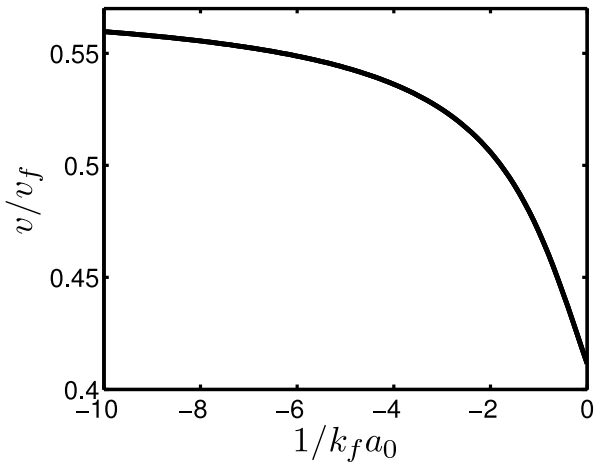

FIG. 7: The speed of sound is shown in units of the Fermi velocity $v_f = \hbar k_f/m$ for an uniform two-component Fermi gas, as a function of $k_f a_0$.

energy functional is:

$$\mathcal{E}(\psi) = \int\left(2\sum_i^{N/2}\psi_i(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2\mathbf{r}^2\right)\psi_i(\mathbf{r}) + \frac{4\pi\hbar^2 k_f a_{eff}(k_f(\mathbf{r})a_0)}{k_f(\mathbf{r})m}\rho(\mathbf{r})^2\right)d\mathbf{r}. \tag{32}$$

In this approximation, the renormalization is done locally, $k_f(\mathbf{r}) = (6\pi^2\rho(\mathbf{r}))^{1/3}$. The minimization procedure is lengthly and straight forward, so it will not be presented here. By minimizing with respect to the set of orbitals ψ_i, we obtain a set of nonlinear HF equations. These are solved self-consistently. Figure 4 shows results for the HF energy of 2280 particles. This approximation is particulary useful for systems with small number of particles, for which the TF approximation has limited applicability. In Sec. IV below, this method is used to obtain the energies of 8 fermions in a trap.

IV. RESULTS

To compare the predictions based on our renormalized scattering length with other methods we have carried out fixed node diffusion Monte Carlo (FNDMC) simulations for equal mixture of different-spin fermions. Interactions are considered only between different-spin fermions, which are treated here as distinguishable particles. The interaction potential is a purely attractive gaussian and its width d is chosen so that $\rho d^3 \approx 10^{-4}$. The method follows closely the approach of [36].

The ground state wavefunction of two particles in a trap can be separated exactly into a Jastrow term and non-interacting orbitals

$$\Psi_p(\mathbf{r_1},\mathbf{r_2}) = \psi(\mathbf{r_1})\psi(\mathbf{r_2})J(\mathbf{r_1}-\mathbf{r_2}), \tag{33}$$

where ψ is the non-interacting ground state orbitals. We will show that this relation is valid when the center of mass wavefunction and the noninteracting orbitals are gaussians, like in the trapped. For this discussion $\hbar = m = \omega = 1$ and we will not consider normalization factors. If we define $\mathbf{R}_{CM} = (1/2)(\mathbf{r_1} + \mathbf{r_2})$ and $\mathbf{r} = (\mathbf{r_1} - \mathbf{r_2})$ we know that the pair wave function can be separated in center of mass and relative coordinate term, $\Psi_p(\mathbf{r_1}, \mathbf{r_2}) = \Psi(\mathbf{R}_{CM})\phi(\mathbf{r})$. Also, we know that the center of mass wavefunction is unaffected by the two-body interaction and is $\Psi(\mathbf{R}_{CM}) = \exp(-\mathbf{R}_{CM}^2) = \exp(-\mathbf{r}_1^2/2)\exp(-\mathbf{r}_2^2/2)\exp(\mathbf{r}^2/4) = \psi(\mathbf{r}_1)\psi(\mathbf{r}_2)\exp(\mathbf{r}^2/4)$, so the total wavefunction is $\Psi(\mathbf{R}_{CM})\phi(\mathbf{r}) = \psi(\mathbf{r}_1)\psi(\mathbf{r}_2)\exp(\mathbf{r}^2/4)\phi(\mathbf{r}) = \psi(\mathbf{r}_1)\psi(\mathbf{r}_2)J(\mathbf{r})$, where $J(\mathbf{r}) = \exp(\mathbf{r}^2/4)\phi(\mathbf{r})$. The evaluation of the relative coordinate wavefunction, $\phi(\mathbf{r})$, requires in general of a numerical calculation.

We use this Jastrow term to construct the many-body wavefunction. This wavefunction is usually called Jastrow-Slater wavefunction. Here, i and i' correspond to different-spin fermions. The non-interacting wavefunction is a Slater determinant formed with the harmonic oscillator orbitals.

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \prod_{ii'} J(\mathbf{r_i} - \mathbf{r_{i'}})\Psi_{NI}(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \tag{34}$$

We have also used a BCS-type many-body wavefunction constructed with pair wavefunctions for FNDMC

$$\Psi(\mathbf{r}_1, \mathbf{r}'_1, ..., \mathbf{r}_{N/2'}) = \mathcal{A}\left\{\Psi_p(\mathbf{r}_1, \mathbf{r}_{1'})\Psi_p(\mathbf{r}_2, \mathbf{r}_{2'})...\Psi_p(\mathbf{r}_{N/2}, \mathbf{r}_{N/2'})\right\}, \tag{35}$$

where $\mathcal{A}$ is the antisymmetrizer operator. This trial wavefunction leads to good results on the BEC limit but in the BCS regime the Jastrow-Slater wavefunction produces lower energies.

We have calculated FNDMC energies for 8 particles in the BCS side of the crossover. In Fig. 8 these energies are compared with HF calculations including the first- and second-order corrections in the $k_f a_0$ expansion [27], and then also with full HF calculations using the renormalized scattering length directly.

$$E_{int}/N = \frac{\hbar^2 k_f^2}{m}\left(\frac{k_f a_0}{3\pi} + \frac{6(11 - 2\ln 2)}{105\pi^2}(k_f a_0)^2 + ...\right) \tag{36}$$

The idea of using this type of expansion to construct energy functionals has been applied for bosons [45, 46]. The expansion (36) can be introduced locally in variational treatments, which yields an energy functional,

$$\mathcal{E}(\psi) = \int \left(2\sum_i^{N/2}\psi_i(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2\mathbf{r}^2\right)\psi_i(\mathbf{r}) + \frac{4\pi\hbar^2 a_0}{m}\rho(\mathbf{r})^2 + a_0^2\frac{12(11 - 2\log(2))}{105\pi^2}(6\pi^2)^{4/3}\rho(\mathbf{r})^{7/3}\right)d\mathbf{r}. \tag{37}$$

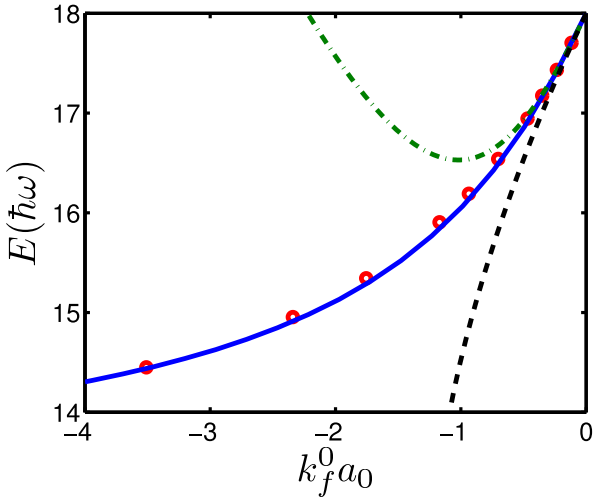

FIG. 8: (Color Online) The total energy of 8 fermions in a trap is shown in oscillator units as a function of $k_f^0 a_0$. FNDMC results are shown in open red circles while full blue line corresponds to HF results using the effective renormalized scattering length. The dashed and the dash-dotted curves correspond respectively to solution use first-order, or first- and second-order terms, in an expansion into powers of $k_f a_0$. See the discussion of Eqs. (36,37).

where $\rho = \rho_\uparrow = \rho_\downarrow$. If we only consider the first term in Eq. 36 we obtain the Fermi pseudo-potential contribution.

To study the weak interacting limit, previous authors [10, 31] have considered the Fermi pseudopotential approximation, which is only the first term in the energy expansion (36). Applying the expansion (36) in the local density approximation is a convenient way to introduce higher order corrections to mean field theories. We can obtain an expansion of the density-dependent renormalization function using Eq. (36), in this case

$$\zeta(k_f a_0) = k_f a_0 + \frac{6(11 - 2\ln 2)}{35\pi}(k_f a_0)^2 + ... \tag{38}$$

Insertion of this result into Eq. (1), with the local density approximation and a Slater determinant wavefunction, gives Eq. (37).

A power expansion of $\zeta(k_f a_0)$ obtained by the renormalization method should agree with this expansion. The first term is reproduced exactly but the second one is only in qualitative agreement. While the coefficient of the second order expansion in Eq. (38) is approximately 0.525, in the density renormalization from Section II the coefficient is 0.422. This disagreement may be due to the level of approximation of the density renormalization procedure.

We find very good agreement between the mean-field results calculated using the renormalized interaction developed in this paper, and the FNDMC (Fig. 8). The variational methods including the perturbative corrections (Eq. 37) show good agreement in the small $k_f a_0$

region, deviating from the FNDNC results when the corrections to the expansion (36) become important.

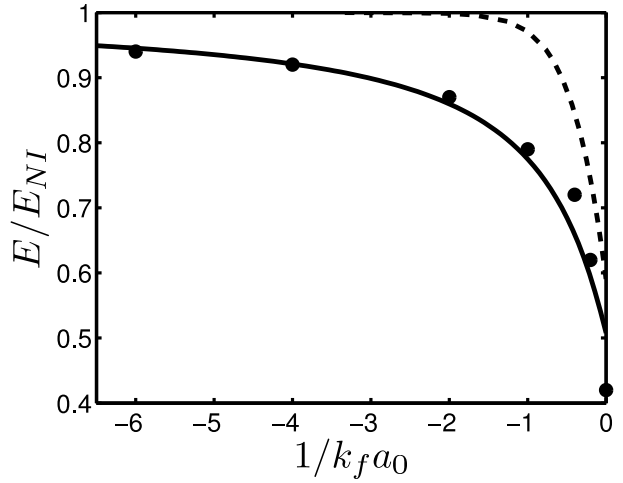

FIG. 9: E/E_{NI} for an infinite homogeneous Fermi gas $k_f a_0$ in the mean-field approach (solid line). The dashed curve corresponds to the local density BCS solution and the circles correspond to FNDMC results obtained in [36].

It is also possible to make comparisons with other quantum Monte Carlo calculations. Astrakharchik and coworkers [36] have studied a homogenous doubly degenerate Fermi gas using FNDMC methods. In their calculations, they considered up to 60 particles. We compare the energy of this system as obtained using the density renormalization procedure in Eq. (24). A comparison between the two calculations and local density BCS result [47, 48] is shown in Fig. (9).

V. CONCLUSIONS

It is the goal of most many-body theoretical studies to derive predictive power for numerous observables of interest, using simpler methods that bypass the actual calculation of this "true" ground state wavefunction for the trapped atomic gas. At the heart of many such treatments are the following two steps: *(i)* replacement of the two-body potential energy by a zero-range Fermi pseudopotential, followed by *(ii)* a mean-field wavefunction ansatz and the computation of observables. The basic level of description for a Bose gas incorporates no correlations whatsoever. For a Fermi gas, correlations are generally treated at either the bare minimalist level of exchange correlations alone, using a single Slater determinantal wavefunction. A more sophisticated level is often considered for a system of mutually attractive fermions, which are frequently described with BCS-type correlations built into the description. One way of visualizing the value of a Fermi-type zero-range pseudopotential adopted in most such theories is to remember that it has been specifically designed to give a meaningful interaction energy for each pair of particles even when the wavefunction structure is too simplistic to incorporate any appreciable correlations.

The present article presented an alternative implementation of this general philosophy. We developed a procedure for renormalizing the coefficient of a zero-range potential, based entirely on an analysis of the nonperturbative two-body system solved first with and then without wavefunction correlations. When we applied this procedure to the many-body Fermi gas, it gives agreement with the standard dilute gas limit, an important prerequisite for any realistic theory. But in addition, it is able to treat higher densities n, including the regime $|n{a_0}^3| >> 1$. We studied a number of observables that have been explored both experimentally and theoretically in the BCS-BEC crossover regime, and found good agreement using our renormalized Hartree-Fock approach all the way to the unitarity limit $a_0 \to \infty$. Perhaps surprisingly, this good agreement is achieved without incorporating explicit BCS-type correlations into the many-body wavefunction. One result of this study is an approximate expression for the renormalization function in closed analytical form that may prove to be useful in other studies of the two-component degenerate Fermi gas. Another interesting result is that at unitarity, the chemical potential exhibits the expected density dependence characterized by the parameter $\beta = -0.492$, which, interestingly, is consistent with recent experiments [1, 2, 3, 4].

In order to study the complete BCS-BEC crossover, future improvements of this theory should include a more flexible many-body wavefunction which can represent a Fermi gas in the weak interacting region and a gas of Bose molecules in the BEC region.

Acknowledgments

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